Naval Research Laboratory

Washington, DC 20375-5320



NRL/MR/6404--97-7918

Adaptive Refinement Tree—A New High-Resolution N-Body Code for Cosmological Simulations

Andrey V. Kravtsov Anatoly A. Klypin

Astronomy Division, New Mexico State University Las Cruces, NM

ALEXEI M. KHOKHLOV

Laboratory for Computational Physics and Fluid Dynamics

February 28, 1997

DTIC QUALITY INSPECTED 4

Approved for public release; distribution unlimited.

19970307 038

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, Including the time for reviewing Instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget. Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE	3. REPORT TYPE A	ND DATES COVERED
	February 28, 1997		
4. TITLE AND SUBTITLE			5. FUNDING NUMBERS
Adaptive Refinement Tree — A for Cosmological Simulations	N0001497WX40001 AST9319970		
6. AUTHOR(S)			
A.V. Kravtsov,* A.A. Klypin,*	and A.M. Khokhlov		
7. PERFORMING ORGANIZATION NAME	(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION REPORT NUMBER
Naval Research Laboratory			ND 0.50 (404 05 5010
Washington, DC 20375-5320			NRL/MR/640497-7918
9. SPONSORING/MONITORING AGENCY	NAME(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING AGENCY REPORT NUMBER
NSF, 4201 Wilson Blvd., Arlin	gton, VA 22230		AGENCT REPORT NOWBER
ONR, 800 North Quincy St., A	_		
11. SUPPLEMENTARY NOTES	-	<u></u>	
Astronomy Department, New M Las Cruces, NM	fexico State University		
12a. DISTRIBUTION/AVAILABILITY STA	TEMENT		12b. DISTRIBUTION CODE
Approved for public release; dis	stribution unlimited.		
			

13. ABSTRACT (Maximum 200 words)

We present a new high-resolution N-body algorithm for cosmological simulations. The algorithm employs a traditional particle-mesh technique on a cubic grid and successive multilevel relaxations on the finer meshes, introduced recursively in a fully adaptive manner in the regions where the density exceeds a predefined threshold. The mesh is generated to effectively match an arbitrary geometry of the underlying density field—a property particularly important for cosmological simulations. In a simulation the mesh structure is not created at every time step but properly adjusted to the evolving particle distribution. The algorithm is fast and effectively parallel: the gravitational relaxation solver is approximately two times slower than the FFT solver on the same number of mesh cells. The required CPU time scales with number of cells, N_c , as $\sim O(N_c)$. It allows us to improve considerably the spatial resolution of the particle-mesh code without loss in mass resolution. We present a detailed description of the methodology, implementation, and tests of the code.

We further use the code to study the structure of dark matter halos in high-resolution ($\sim 2h^{-1}$ kpc) simulations of standard CDM ($\Omega=1,\ h=0.5,\ \sigma_8=0.63$) and Λ CDM ($\Omega_{\Lambda}=1-\Omega_0=0.7,\ h=0.7,\ \sigma_8=1.0$) models. We find that halo density profiles in both CDM and Λ CDM models are well fit by the analytical model presented recently by Navarro et al. (1966) which predicts a singular ($\rho(r) \propto r^{-1}$) behavior of the halo density profiles at small radii. We therefore conclude that halos formed in the Λ CDM model have structure similar to the CDM halos, and thus cannot explain dynamics of the central parts of dwarf spiral galaxies inferered from their rotation curves.

14. SUBJECT TERMS	15. NUMBER OF PAGES		
Methods Cosmology Numerical Theory—dark matter			40
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

CONTENTS

1.	INTRODUCTION	1
2.	METHODOLOGY	2
	2.1 Adaptive Mesh Refinement	2
	2.2 Multilevel Relaxation Method	3
3.	DESCRIPTION OF THE CODE	3
	3.1 Code Structure	3
	3.2 Mesh Generator	4
	3.3 Particles within the Mesh Hierarchy and Density Assignment	6
	3.4 Poisson Solver	6
	3.5 Particle Dynamics	8
	3.6 Parallelization	9
	3.7 Memory Requirements	9
	3.8 Timing	10
	3.9 Energy Conservation	11
4.	TESTS OF THE CODE	12
	4.1 Force Accuracy	12
	4.2 Zel'dovich' Pancake Collapse	13
	4.3 Spherical Infall Test	13
	4.4 Realistic Cosmological Runs: Comparison with PM Code	14
5.	AN APPLICATION STRUCTURE OF DARK MATTER HALOS	
	IN CDM AND ACDM MODELS	15
	5.1 Motivation	15
	5.2 Simulations	16
	5.3 Halo Finding Algorithms	16
	5.4 Results: Halo Density Profiels	17
	5.5 Effects of Resolution	18
	5.6 Conclusions	18
6.	DISCUSSION AND CONCLUSIONS	18
DE	EEDENCES	10

ADAPTIVE REFINEMENT TREE - A NEW HIGH-RESOLUTION N-BODY CODE FOR COSMOLOGICAL SIMULATIONS

1. Introduction

N-body techniques are used in cosmological simulations to follow the non-linear evolution of a system of particles, and to give theoretical predictions about the matter distribution which can be compared with observations. The traditional N-body methods are Particle-Mesh (PM), Particle-Particle/Particle-Mesh (P³M), and TREE (Hockney & Eastwood 1981; Klypin & Shandarin 1983; Efstathiou et al. 1985; Bouchet & Hernquist 1988; and references therein). Although these algorithms proved to be useful, with currently available computers all of them fall short of the spatial or mass resolution desired in cosmological simulations. For example, one needs a resolution $\sim 1-10$ kpc to resolve a galaxy and a simulation cube of ~ 100 Mpc to sample appropriately the longest perturbation waves or to get sufficient statistics. The required dynamical range is thus $\sim 10^4-10^5$ which is much higher than current codes can allow. These limitations have motivated the development of new methods with better resolution and/or performance.

Villumsen (1989) developed a code where the PM grid was complemented by finer cubic subgrids to increase the force resolution in regions of interest. The local potential was calculated as a sum of the potentials on the subgrids and on the PM grid. A similar approach was adopted by Jessop, Duncan & Chau (1994) in their particle-multiple-mesh code. However, instead of summing the potentials from subgrids, the potential on each level was obtained independently by solving the boundary problem. Boundary values of the potential were interpolated from the coarser parent grid. Couchman (1991) used cubic refinement grids to improve the performance of the P3M algorithm. Here, the resolution was retained at the level of the P³M code while the computational speed was considerably increased. In the Lagrangian approach (Gnedin 1995; Pen 1995) the computational mesh is not static but moves with the matter so that the resolution increases (smaller mesh cells) in the high density regions and decreases elsewhere. Although potentially powerful, this approach has its caveats and drawbacks (Gnedin & Bertschinger 1996). The mesh distortions, for example, may introduce severe force anisotropies. A different approach was adopted by Xu (1995), who developed the TPM code - a hybrid of the PM and TREE algorithms. The gravitational forces in the TPM are calculated via a PM scheme on the grid and via multipole expansions (TREE algorithm) in the regions where higher force resolution is desired. The forces on the particles in low-density regions are calculated by the PM scheme, while forces on the particles in high-density regions are sum of external large-scale PM force and internal short-scale force from the neighboring particles. Although this code may not be faster than a pure TREE code, it is effectively parallel because particles in different regions can be evolved independently. An adaptive multigrid code for cosmological simulations was recently presented by Suisalu & Saar (1995). In this code, finer rectangular subgrids are adaptively introduced in regions where the density exceeds a specified threshold. For each subgrid the potential is calculated using boundary conditions interpolated from the coarser grid. The solution on the finer grid is used to improve the solution on the coarser grid. Another variant of an adaptive particle-multiple-mesh code for cosmological simulations was recently presented by Gelato, Chernoff, & Wasserman (1996). This code can handle isolated boundary conditions which makes it applicable to non-cosmological problems.

All of the above multigrid methods use rectangular subgrids to increase force resolution. For simulations where there are only a few small regions of interest (e.g., a few galaxies or clusters of galaxies) the rectangular refinements may be a good choice because these regions can be easily covered by rectangular subgrids. It is, however, well-known that the geometry of structures in realistic cosmological models is usually a complicated network of sheets, filaments, and clumps which are difficult to cover efficiently with rectangular grids.

In this paper we present a new Adaptive Refinement Tree (ART) high-resolution N-body code. This code was developed to improve the spatial resolution of particle-mesh code by about two orders of magnitude

without loss in mass resolution and computational speed. In our scheme, the computational volume is covered by a cubic rectangular grid which defines the minimum resolution. On this grid, the Poisson equation is solved with a traditional Fast Fourier Transform (FFT) technique using periodic boundary conditions. The finer meshes¹ are built as collections of cubic, non-overlapping cells of various sizes organized in *octal threaded trees* in regions where the density exceeds a predefined threshold. Any mesh can be subject to further refinements; the local refinement process stops when density criterion is satisfied. Once constructed, the mesh is not destroyed at every time step but promptly adjusted to the evolving particle distribution. To solve the Poisson equation on these refinement meshes, we use a relaxation method with boundary conditions and initial solution guess interpolated from the previous coarser mesh. Below we present the method (Section 2), describe the code (Section 3), and discuss the tests (Section 4). We then compare the code with other algorithms (Section 4), and finally apply it to a real cosmological problem (Section 5).

2. Methodology

2.1. Adaptive mesh refinement

Adaptive mesh refinement (AMR) techniques for solving partial differential equations (PDEs) have numerous applications in different fields of physics, astrophysics, and engineering where large dynamic range is important. There are two major approaches in application of these techniques. In the first approach (e.g., Berger & Oliger 1984; Berger 1986; Berger & Colella 1989), the computational volume is divided in cubic elements (cells), while in the second (e.g., Löhner & Baum 1991) the cells can have an arbitrary shape. Collections of cells are used as computational meshes on which the PDEs are discretized. We will call meshes composed of cubic cells regular, calling meshes irregular otherwise. The integration of PDEs is simpler on regular meshes but dealing with complicated boundaries may be a difficult problem. With irregular meshes one can handle complicated boundaries much more easily. The price, however, is more elaborate algorithms, data structures, and associated CPU and memory overhead. A particular choice of the mesh structure is a tradeoff between these considerations. In astrophysics there are no complicated boundaries, and a cubic computational volume is usually used to model a system. In this case, there is no need in irregular meshes and it is preferable to use meshes made of cubic cells.

The regular meshes themselves can be organized in different ways. The usual practice is to use regular meshes of cubic or rectangular shape (e.g., Berger & Colella 1989) organized in arrays (grids). This allows one to simplify data structures and to use standard PDE solvers. These arrays can be organized in a tree (Berger 1986) to form a multigrid hierarchy. The main disadvantage of the grids is that one cannot cover regions of complicated shape in an efficient way. Moreover, the arrays are unflexible data structure, and the whole refinement hierarchy should be periodically rebuilt, not adjusted, when dealing with unsteady solutions.

In our approach, we use regular meshes but they are handled in a completely different way. Cells are treated as individual units which are organized in refinement trees (see Section 3.2). Each tree has a root – a cell belonging to a base cubic grid which covers the entire computational volume. If the root is refined (split) – it has 8 children (smaller non-overlapping cubic cells residing in its volume) which in their turn can be refined, and so on. Cells of a given refinement level are organized in linked lists and form a refinement

¹We will use word *grid* to refer to the cubic or rectangular configurations, reserving the word *mesh* for configurations of arbitrary shape.

mesh. The tree data structures make mesh storage and access in memory logical and simple, while linked lists allow for efficient mesh structure traversals. In the current version of the code we make use of octal threaded trees (Khokhlov 1997) and doubly linked lists (e.g., Knuth 1968; Aho, Hopcroft, & Ulman 1983; Corner, Leiserson, & Rivest 1994). The fact that cells are treated as independent units rather than element of a grid allows us to build a very flexible mesh hierarchy which can be easily modified. The details of the mesh generation and modification in our code are described in Section 3.

2.2. Multilevel relaxation method

The multigrid techniques of solving partial differential equations (Brandt 1977) are very successful in reducing the computational and storage requirements for solving many types of PDEs (Wesseling 1992, Press et al. 1992). There are two kinds of multigrid algorithms. The first, sometimes called multigrid method, is used to speed up convergence of relaxation method. In this method, the source term is defined only on the base finest grid – all the other coarser grids are used as a workspace. In the second algorithm, called full multigrid, the source term is defined on all grids, and the method obtains successive solutions on finer and finer grids. The latter method is useful when dealing with grids created in adaptive refinement process. The full multigrid scheme in its turn can be used differently depending on how the solutions on different levels influence each other. In the one-way interface scheme, the solution from a coarser grid is used to get a first guess solution on the finer grid, and often to get boundary values as well. However, the solution on the coarser grid is not influenced by the solution on the finer grid (e.g., Jessop, Duncan, & Chau 1994). In the two-way interface scheme, the coarser grid solution is used to correct the solution on the finer grids and vice-versa. The choice of a particular scheme is usually determined empirically, and is problem dependent. The two-way interface scheme is more difficult to implement in the case of periodic boundary conditions (Suisalu & Saar 1996).

In our approach, each refinement mesh is composed of cells of the same refinement level but these meshes are completely different from grids. The techniques are thus multilevel rather than multigrid. We use an analog of full multigrid algorithm with the one-way interface between the meshes. We use a regular cubic grid covering the whole computational volume as the zeroth, coarsest level. At this level, the Poisson equation is solved using a standard FFT method with periodic boundary conditions. This solution is then interpolated on to the first level finer mesh to get the boundary values and first solution guess. Once the boundary problem is defined, we use a relaxation method (e.g., Press et al. 1992) to solve the Poisson equation on this mesh. As we start from an initial guess which is already close to the final solution, the iterative relaxation procedure converges fast. After we get the solution on the first refinement level, the same procedure (obtaining boundary values and initial guess by interpolation from the previous coarser level) is repeated for the next level, and so forth. At the end of this process we have the solution (potential) for all cells. The description of the code is given in the next section.

3. Description of the code

3.1. Code structure

The structure of the code can be outlined as follows. First of all, we set up the initial positions and velocities of the particles using the Zel'dovich approximation as described by Klypin & Shandarin (1983). Once the initial conditions are set we construct the regular cubic grid covering the whole computational

volume and then proceed to check if additional refinement levels are required according to the current density threshold. At this point the code enters the main computational loop which includes:

- density assignment on all existing meshes;
- gravitational solver;
- routine updating particle positions and velocities;
- · modifications to the mesh hierarchy.

The mesh modifications (refinement and derefinement) are based on the density distribution². The modifications are made at the end of the computational cycle. At this point the density distribution is available (it was calculated for the gravitational solver).

Below we will describe each of these major functional blocks in detail. We will also discuss memory requirements of the code, timing, and energy conservation.

3.2. Mesh generator.

The adaptive mesh refinement block of the code generates new and modifies existing meshes. The refinement hierarchy in our implementation is based on the regular cubic grid which covers the entire computational volume. With the refinement block turned off, the density assignment and gravity solver on this grid are similar to those in the PM code of Kates, Kotok, & Klypin (1991).

The data structures that we use to organize the mesh cells are very similar to those implemented in the hydrodynamical Eulerian Tree Refinement code³ (Khokhlov 1997). All mesh cells are organized in refinement trees. A cell can be a parent of eight children – smaller cubic cells of equal volume residing in it. Each child may be in its turn split and have children. Each tree has a root – a zero level cell – which may be the only cell in this tree if it is unsplit. The tree ends with unsplit cells, which we call leaves. This structure is called an octal rooted tree – the construct which is used in TREE codes. There is, however, an important difference. We use fully threaded trees, that is trees which are connected with each other on all levels⁴. Note, that we can consider all cells as belonging to a single threaded tree with a root being the entire computational domain and the base grid being one of the tree levels. The tree structure is supported through a set of pointers. Each cell has a pointer to its parent and a pointer to its first child. In addition, cells has pointers to the six adjacent cells (these make the tree fully threaded) so that information about cell's neighbors is easily accessible (see Fig.1). Overall, the following information is provided for each cell i belonging to a tree:

- Level(i) level of the cell in the tree;
- Parent(i) pointer to the parent cell;

²The density criterion in our case is a natural choice because we aim to resolve high density regions. We could use, however, any other appropriate criterion, e.g. local potential gradient, force accuracy etc.

³There are, however, some important modifications which were required by specifics of the cosmological simulations.

⁴In simple threaded trees only leaves are connected.

- Child(i) pointer to the cell's first child or nil if the cell is a leaf;
- Nb(i, j) pointers to the neighbors $(j = 1 \rightarrow 6)$;
- Pos(i, j) position in space $(j = 1 \rightarrow 3)$;
- Var(i, n) storage for associated physical variables (in our case n = 2, as we keep both density and potential).

The above set of pointers is sufficient to support the tree structure and to change it dynamically with minimum cost. In addition, the cells on each level of the mesh hierarchy are organized in doubly linked lists⁵ (e.g., Knuth 1968) so that a sweep through a given level (the operation used extensively in multigrid relaxations described below) can be done with minimum CPU time. The cells belonging to the base regular grid (level zero), while part of the same data structure, are created only at the very beginning of a simulation and are never destroyed. It is therefore unnecessary to keep information about a cell's position or pointers to its neighbors because they can be easily computed. The number of pointers can be considerably reduced (by as much as a factor of 2) because some of them can be shared by siblings (the eight cells which have the same parent).

An elementary refinement process creates 8 new cubic cells of equal volume (children) inside a parent cell. When the parent is refined, we check if all six neighbors are of the same level as the parent. If there are neighbors of smaller level (coarser) than the parent, we split them. If a neighbor in its turn has coarser neighbors, we split the neighbor's neighbors, and so forth. We thus build a refinement structure which obeys a rule allowing no neighbor cells with level difference greater than 1. Examples of allowed and prohibited configurations are shown in Fig.2. Although this is the only rule in the whole refinement process, it determines the global structure of the resulting refinement hierarchy assuring that on a level's boundaries there are no sharp resolution gradients. On the next refinement pass each of the newly born children is checked against the density criterion and can be in its turn subdivided into 8 children if further splitting is needed. The process stops when either the density criterion is satisfied everywhere or the maximum allowed refinement level is reached.

The refinement process proceeds level by level starting from the base grid. On any level of the mesh hierarchy the process can be split into two major parts. First, we mark up⁶ all the cells which need to be split creating a refinement map. However, the map constructed this way tends to be "noisy". We smooth it by marking additional cells so that any cell which was marked originally is surrounded by a buffer of at least two other marked cells. We construct this buffer using an algorithm which includes several passes through a level, each one marking additional cells. During the first pass the neighbors of cells marked in the refinement map are marked for splitting also. After that, two passes are made in which we mark for splitting only those cells which have at least two neighbors already marked for refinement (note, that we mean cells marked during all previous (not the current) passes). These three passes create a one-cell cubic buffer around each of the cells marked in the original refinement map. Each additional set of three passes similar to those described above will build one more cubic layer around every originally marked cell. Therefore, to build a two-cell buffer we make six passes. When the map is completed, it is used to make the actual splitting.

⁵The difference between a doubly linked list and the usual linked list (used, for example, in the P³M codes) is that in the former we keep not only a pointer to the next element but also a pointer to the previous element in the list. This allows us to insert and delete list entries without rebuilding the whole list.

⁶A cell is marked for splitting when the local density exceeds a predefined level-dependent threshold.

The refinement procedure described above can be used either to construct the mesh hierarchy from scratch or to modify the existing meshes. However, in the course of a simulation the structure is neither constructed nor destroyed. Instead, on every computational cycle we modify existing meshes to account for the changes in particle distribution. Therefore, we need to make not only refinements but also derefinements (in the places where it is no longer necessary to keep resolution at the current level) which is done in the same manner by constructing a derefinement map – that is, map of cells marked for joining. If the joining violates the above mentioned neighbor rule nothing is done and the cell is kept split. Therefore, the code modifies the existing structure dynamically keeping the refinements in accord with the ever changing density field. The modification of the hierarchy requires much less CPU time than rebuilding it because only a small number of cells needs to be modified at any given time step. Fig.3 shows an example of the refinement mesh hierarchy built in one of the Λ CDM cosmological simulations described in Section 4.4

3.3. Particles within the mesh hierarchy and density assignment

Particle coordinates are not sufficient to specify the particle-mesh connection because cells of different levels can share the same volumes. We need to know, however, which particles belong to a given cell. This is done by arranging particles in doubly linked lists so that every cell "knows" its head linked list particle (the head is nil if the cell is empty) and thus all the other particles in this linked list. If a particle moves from cell to cell, it is deleted from the linked list of the cell it leaves and is added to the new cell's linked list. Only leaves are allowed to own particles. Once a cell is split, all its particles are divided among its children. However, we solve the Poisson equation on every refinement level so that the density is needed in every cell regardless of whether or not it is a leaf. On each level, starting from the finest and up to the level zero, the density is assigned using the standard Cloud-In-Cell (CIC) technique (Hockney & Eastwood 1981). Because particles belong only to the finest cells enclosing them, when we go from level to level the particles are passed from children to their parents. This is done only for the density assignment and the linked list is not changed. The particles, therefore, contribute to the density on any level they are physically located on.

3.4. Poisson solver

The fact that level zero of the mesh hierarchy is a cubic regular grid of fixed resolution allows us to use the FFT method to solve the Poisson equation on this grid (Hockney & Eastwood 1981). The FFT technique naturally supports periodic boundary conditions which is important for cosmological simulations.

The Poisson equation on the refinement meshes is defined as a Dirichlet boundary problem where boundary values are obtained by interpolating the potential from the parent grid. In our algorithm, the boundaries of the refinement meshes can have an arbitrary shape which narrows the range of PDE solvers that one can use. To solve the Poisson equation on these meshes, we have chosen the relaxation method (Hockney & Eastwood 1981; Press et al. 1992). It is relatively fast and efficient in dealing with complicated boundaries. In this method the Poisson equation

$$\nabla^2 \phi = \rho \tag{1}$$

is rewritten in the form of a diffusion equation,

$$\frac{\partial \phi}{\partial \tau} = \nabla^2 \phi - \rho,\tag{2}$$

or, in finite difference form:

$$\phi_{i,j,k}^{n+1} = \phi_{i,j,k}^{n} + \frac{\Delta \tau}{\Delta^2} \left(\sum_{nb=1}^{6} \phi_{nb}^{n} - 6\phi_{i,j,k}^{n} \right) - \rho_{i,j,k} \Delta \tau.$$
 (3)

where the summation is performed over a cell's neighbors. Here, Δ is the actual spatial resolution of the solution (potential), while $\Delta \tau$ is a fictitious time step (it is not related to the actual time integration of the N-body system). This finite difference method is stable when $\Delta \tau \leq \Delta^2/6$ (Press et al. 1992). If we choose the maximum allowed time step $\Delta \tau = \Delta^2/6$, the above equation can be rewritten in the form of the following iteration formula:

$$\phi_{i,j,k}^{n+1} = \frac{1}{6} \left(\sum_{n_b=1}^6 \phi_{n_b}^n - 6\phi_{i,j,k}^n \right) - \frac{\Delta^2}{6} \rho_{i,j,k}. \tag{4}$$

The relaxation iteration is thus averaging the potential of a cell's six neighbors and subtracting the contribution from the source term. Cells in the boundary layer will have some neighbors belonging to the coarser level. In this case, we need to interpolate to get the potential at the location of the expected neighbor. It is desirable that the interpolation maintain continuity and isotropy of the force (see discussion in Jessop et al. 1994). We have found that linear interpolation perpendicular to the boundary which incorporates both coarser and finer cell potentials is satisfactory; we get the interpolated value of the potential on the boundary of level l as:

$$\phi_{int} = w_i \phi_l + (1 - w_i) \phi_{l-1}. \tag{5}$$

Here w_i is a weight, and ϕ_l and ϕ_{l-1} are the potentials of a boundary cell of level l and of its (l-1)-level neighbor. We have found the optimal value of w_i to be 0.2 by minimizing the force discontinuity for particles moving through mesh boundaries. The iterative procedure described above is then repeated until the desired level of convergence is achieved. We can considerably speed-up the convergence of the relaxation procedure by using an initial guess for the solution which is already close to the final solution. Such an initial guess can be obtained by interpolating the potential from the previous coarser mesh, where the Poisson equation was already solved. By doing so, we need only 2-3 iterations to get the potential with an accuracy of a couple per cent. Nevertheless, a higher accuracy is needed because the potential is then differentiated to get the accelerations and the errors in accelerations are thus larger than errors in the potential. Therefore, we would need to make more iterations to reach the same $\sim 1-2\%$ accuracy level. The number of required iterations, however, can be considerably reduced by using the so-called Successive Overrelaxation (SOR) technique (Hockney & Eastwood 1981; Press et al. 1992). In this technique the solution in a given cell is computed as a weighted average,

$$\phi_{*}^{n+1} = \omega \phi^{n+1} + (1 - \omega)\phi^{n}, \tag{6}$$

where ϕ^{n+1} is the solution obtained via the iteration equation (4), ϕ^n is the solution from previous iteration step, and ω is the overrelaxation parameter. The parameter ω can be adjusted to minimize the number of iterations required to achieve a certain accuracy level. Of course, there is no point in using more iterations than is needed to make the iteration error smaller than truncation error. The latter can be estimated by making the number of iterations very large so that the iteration error is negligible.

The ultimate goal of any N-body algorithm is to get an accurate approximation to the pairwise interparticle forces. Therefore, we use the force accuracy (see Section 4) to determine the required number of iterations. We do this by adjusting the overrelaxation parameter ω to minimize the number of iterations while keeping the force accuracy at the level of truncation errors. We have found empirically that only 10 relaxation iterations is needed if $\omega = 1.25$.

3.5. Particle dynamics

To integrate the trajectories of the dark matter particles we use the Newtonian equations of motion in an expanding cosmological framework (e.g., Peebles 1980). These equations can be expressed in terms of comoving coordinates x related to the proper coordinates as r = a(t)x, where $a(t) = (1+z)^{-1}$ is the expansion factor:

$$\frac{d\mathbf{p}}{dt} = -\nabla_x \phi, \quad \frac{d\mathbf{x}}{dt} = \frac{\mathbf{p}}{a^2},\tag{7}$$

where **p** is the momentum of a particle and $\nabla_x \phi$ is given by the Poisson equation relating the potential ϕ to deviations of density from the background:

$$\nabla_x^2 \phi = 4\pi G a^2 (\rho - \overline{\rho}). \tag{8}$$

The above equations are integrated numerically using dimensionless variables

$$\mathbf{x} = x_0 \widetilde{\mathbf{x}}, \ t = \widetilde{t}/H_0, \ \phi = \widetilde{\phi}(x_0 H_0)^2, \ \mathbf{p} = \widetilde{\mathbf{p}}(x_0 H_0), \ \rho = \widetilde{\rho} \frac{3H_0^2}{8\pi G} \frac{\Omega_M}{a^3}, \tag{9}$$

where x_0 is the length of a zero level mesh cell and H_0 is the Hubble constant. We also use the expansion factor a instead of the time t so that equations (7)–(8) can be rewritten as:

$$\frac{d\tilde{\mathbf{p}}}{da} = -f(\Omega_M, \Omega_\Lambda, a) \, \tilde{\nabla} \tilde{\phi},
\frac{d\tilde{\mathbf{x}}}{da} = f(\Omega_M, \Omega_\Lambda, a) \, \frac{\tilde{\mathbf{p}}}{a^2},
\tilde{\nabla}^2 \tilde{\phi} = \frac{3\Omega_M}{2a} (\tilde{\rho} - 1).$$
(10)

Here Ω_M is the present day (z=0) contribution of matter to the total density of the universe and Ω_{Λ} is the corresponding contribution of the vacuum energy (measured by the cosmological constant). The function f is specific to a given cosmological model. The general form of this function, valid for open, flat, and closed cosmologies, is (e.g. Carrol et al. 1992):

$$f(\Omega_M, \Omega_\Lambda, a) = \frac{1}{\sqrt{1 + \Omega_M (1/a - 1) + \Omega_\Lambda(a^2 - 1)}}.$$
 (11)

We adopt a standard second-order leap-frog integration scheme of advancing particles to the next time step. For a step n, corresponding to time step $a_n = a_{init} + n\Delta a$, the momenta and positions of particles are updated as follows:

$$\widetilde{\mathbf{p}}_{n+\frac{1}{2}} = \widetilde{\mathbf{p}}_{n-\frac{1}{2}} - f(\Omega_{M}, \Omega_{\Lambda}, a_{n}) \widetilde{\nabla} \widetilde{\phi}_{n} \Delta a,$$

$$\widetilde{\mathbf{x}}_{n+1} = \widetilde{\mathbf{x}}_{n} + f(\Omega_{M}, \Omega_{\Lambda}, a_{n+\frac{1}{2}}) \frac{\widetilde{\mathbf{v}}_{n+\frac{1}{2}}}{a_{n+\frac{1}{2}}^{2}} \Delta a.$$
(12)

Here indices n, n+1, and $n\pm\frac{1}{2}$ refer to quantities evaluated at a_n , a_{n+1} , and $a_n\pm\Delta a/2$ respectively. Although multiple time stepping is probably very efficient in terms of CPU time, in the current version of the code we use a constant time step for all particles. We plan to implement individual time steps for different levels in the future. Particle coordinates and velocities are updated using their accelerations obtained via numerical differentiation of the potential and the consequent interpolation to the particle location using

the CIC method (Hockney & Eastwood 1981). There are, however, some complications because particles can move through the level boundaries. The resolution gradients, for example, may induce unwanted force fluctuations and anisotropies (Jessop et al. 1994; Anninos, Norman, & Clarke 1994). In addition, momentum conservation, achieved by exact cancellation of numerical terms in the CIC method, is no longer guaranteed. This means that additional care must be taken to minimize these effects. Usually, this is done by introducing extra buffer regions along the mesh interfaces so that force interpolation on the boundaries is avoided. In our code, we do not introduce additional buffer cells on the mesh boundaries because the meshes are already expanded by smoothing (see Section 3.2). Therefore, we simply prohibit force interpolation that uses both coarse and fine boundary cells, interpolating instead on the coarse level. In this way, particles are driven by the coarse force until they move sufficiently far into the finer mesh. The same is true for particles moving from the finer to coarser mesh.

3.6. Parallelization

The success of a numerical algorithm largely depends on how easily it can be parallelized to run on large multiprocessor computers. The parallelization strategies are problem dependent and are different for shared and distributed memory machines. Here we briefly outline the parallelization specifics of the ART code.

Functionally, the code can be decomposed in two parts – the PM part working on the base grid and the part dealing with refinement meshes. The PM algorithm was successfully parallelized for both massively parallel distributed memory (such as CM-5 (Ferrell & Bertschinger 1994; Smith 1995) or SP-2 (Gross 1997)) and shared memory machines (Yepes et al. 1996). To be ported to distributed memory systems the ART code requires more elaborate functional and data organization (Khokhlov 1997) but is relatively straightforward to parallelize for shared memory architectures. The most CPU expensive parts of the code – Poisson solver and force interpolation – are effectively parallel. In the mesh modification routine the most expensive part – the construction of refinement and derefinement maps – is also parallel. Currently, blocks of the code that require considerable parallelization efforts but are relatively CPU inexpensive – the density assignment and cell splitting/joining during the mesh modifications⁷ – are run serially.

The present version of the code was parallelized to run in shared memory mode on the HP-Convex SPP-1200 Exemplar – a multi-purpose scalable parallel computer. The timing and benchmarking was performed for one of the simulations described in Section 3.8.

3.7. Memory requirements

Memory requirements of the code are determined by the number of dark matter particles N_p , number of cells in zero level base grid N_c^0 , and number of cells on refinement levels N_c^L . In the current implementation of the code the total number of memory storage elements N used by the code is:

$$N^{ART} \approx 9N_p + 6N_c^0 + 15N_c^L. {13}$$

The overhead for N_c^L is determined by the pointers that are used to support the tree refinement hierarchy (see Section 3.2). It can be reduced by a factor of $\sim 2-3$, if some of the pointers will be shared by siblings

⁷Although the cell splitting and joining procedure is serial, it takes a negligible amount of CPU time because we need to do it only for a small number of cells on each time step.

(the eight cells which have the same parent). The overhead can be reduced even further (making number of storage elements per refinement cell only ~ 2.5) by incorporating more elaborate ideas (Khokhlov 1997). The estimated memory requirement for an optimized code is:

$$N_{opt}^{ART} \approx 9N_p + 4N_c^0 + 4.5N_c^L.$$
 (14)

We plan to implement these improvements in the future versions of the code.

The N^{ART} can be compared to the corresponding number of storage elements in a PM code:

$$N^{PM} \approx 6N_p + N_c^0; \tag{15}$$

The apparent overhead of the ART code compared to PM is the price for fully adaptive and flexible mesh structure. It should be noted, however, that to increase resolution by a factor of 2 in a PM code the number of cells N_c^0 must be increased by a factor of 8 which severely limits the maximum possible dynamic range (which with largest currently available computers is ~ 1000). In the ART code, the resolution is improved by increasing N_c^L which changes very slowly when resolution is increased. For example, to increase resolution in the highest density regions by a factor of 2 in the simulations described in Section 5 (see also Table 1), the total number of cells was increased only by ~ 3%. Note also that the dynamic range of ~ 4000 was achieved with only ~ 5×10^6 cells while a PM code would require ~ 6.4×10^{10} cells to reach the same resolution. For comparison, the memory requirements of the publicly available versions (kindly provided by J.Barnes and H.M.P.Couchman) of TREE code and AP³M code are $N^{TREE} \approx 11N_p + 18N_{cells}$, where N_{cells} is the number of tree cells, and $N^{AP^3M} \approx 13N_p + 2N_c^0$ (not including the overhead related to the refinement meshes in N^{AP^3M}).

3.8. Timing

In this section we present timings of the current version of the code and compare the performance with other high-resolution N-body codes. In Fig.5a we show the performance of different blocks of the code with respect to the expansion parameter in a Λ CDM simulation ($\Omega_{\Lambda} = 1 - \Omega_{0} = 0.7$, h = 0.7, $\sigma_{8} = 1.0$) of an $L = 15h^{-1}$ Mpc box with $N = 32^{3}$ particles and 64^{3} base grid (more details are given in Section 4.4). The simulation was run on 8 CPUs of the NCSA SP-1200 Exemplar in shared memory mode. The CPU overhead for running code in parallel is about 50% and the same simulation run on an IBM RS/6000 workstation performs ~ 2.5 times faster (in terms of CPU but not in terms of wallclock time!). The overhead is mostly due to the unusually large penalty for cache missing events which results if memory is accessed randomly. In Table 1 we present timing for different code blocks for the final time step (z = 0) of two similar Λ CDM simulations with 64^{3} particles (see section 5.2) and with different resolutions. The base grid

Table 1. Code timings for ΛCDM simulations with 64³ particles on 8 CPUs of the SPP-1200 Exemplar.

Routine	Maximum level	Number of mesh cells	Density assignment	FFT solver	Relaxation solver	Particle motion	Mesh modifications	Total
CPU1 (sec)	4	4860976	25.8	26.2	54.5	34.8	44.0	227.3
CPU2 (sec)	6	5019136	30.6	26.4	82.7	40.8	55.7	285.9

in both simulations was 1283 and numbers of the maximum allowed refinement levels were 4 and 6. As before, the simulations were run on 8 CPUs of the SPP-1200 Exemplar. We compare the timings from Table 1 with the performance of the AP3M code (Couchman 1991). The final step in a two level AP3M simulation of an open ($\Omega_0 = 0.5$, $\Omega_{\Lambda} = 0$, h = 0.63, $\sigma_8 = 1.2$) cosmology (box $L = 150h^{-1}$ Mpc, 128^3 grid, 128^3 particles, and smoothing kernel $\eta = 0.1$ cell giving a dynamic range of about 1000) took 1316 CPU seconds on one processor of IBM SP-2 computer (S.Borgani 1996, private communication). This number is roughly consistent with timings presented in original paper of Couchman (1991) if we account for the difference in MFLOPs between used machines. The first simulation in Table 1 is comparable in spatial resolution to the above AP3M simulation but we have to account for the different number of particles. Only density assignment and particle motion directly scale with number of particles. We, therefore, multiply the CPU time spent by these routines by 8 which gives a total time for the final step ~ 650 CPU seconds. Note, however, that about half of this CPU time is penalty for the cache missings which would be negligible for a serial run on the SP-2. The ART code, therefore, is about 3 times faster than AP3M code of comparable resolution. Note also that although in the second simulation from Table 1 the resolution was increased by a factor of 4, the CPU time does not change significantly because only a relatively small number of additional cells was required to resolve the highest density regions.

3.9. Energy conservation

In an expanding Universe, energy conservation is expressed by the Irvine-Layzer-Dmitriev-Zel'dovich equation:

$$\frac{d}{dt}\left[a(T+U)\right] = -T\frac{da}{dt},\tag{16}$$

or

$$a(T+U)|_{a_0}^a = -\int_{a_0}^a T da. {17}$$

Where

$$T = \frac{1}{2} \sum_{i=1}^{N_p} \frac{p_i^2}{a^2}, \quad U = \frac{1}{2} \sum_{i=1}^{N_p} \phi_i.$$
 (18)

The error in energy conservation at a time a_i is then measured by comparing the change in total energy with the change in aU:

$$Error = \frac{a(T+U)|_{a_0}^{a_{i-1}} + \int_{a_{i-2}}^{a_{i-1}} Tda}{aU|_{a_0}^{a_{i-1}}}$$
(19)

In Fig. 5b we show the energy conservation error versus expansion parameter a for two Λ CDM simulations with 32³ and 64³ particles. In both simulations the time step, Δa , was chosen so that all the particles would move not more than a fraction ($\sim 0.1-0.3$) of the mesh cell they are residing in. We note that energy is conserved at the level of $\sim 2\%$ in the 32³ particle simulation and at the level of $\sim 1\%$ in the 64³ particle simulation. The maximum error of $\sim 5\%$ and $\sim 3\%$ for the two simulations occurred when the first two refinement levels were opened at $a \sim 0.18$. This may be a result of the rather fast change in resolution in the regions of ongoing nonlinear collapse.

4. Tests of the code

In this section we present tests of the developed code. Particularly, we show results describing the accuracy of the force calculation in ART scheme and related issues of resolution. We discuss the results of the Zel'dovich pancake test and of the spherical infall test. Finally, we compare results for a set of realistic cosmological runs obtained with ART and PM code.

4.1. Force accuracy

It is important to know the shape and accuracy of both short- and long-range forces, when the resolution of different codes is compared. Here we present a test showing the accuracy of force calculations in PM and ART schemes and compare them to the Plummer softened force which is often used in both P³M and TREE codes.

We used a 64³ base grid with a massive particle in the center and a second particle placed randomly nearby. The refinement meshes were constructed up to the specified level, so that both particles were located on this level. The usual potential and force calculations (described above) were then performed to get the pairwise force between these two particles which was compared with the "exact" Newton force. Fig. 6 shows the results of the force calculation with the FFT method (i.e., ART without refinements) and with the relaxation method at different levels of refinement. We plot relative acceleration errors calculated as follows:

$$Error = \frac{|\mathbf{a}_{calc}| - |\mathbf{a}_{theor}|}{|\mathbf{a}_{theor}|},$$

where $|a_{calc}|$ is the acceleration calculated on the mesh and $|a_{theor}|$ is the theoretical acceleration. The upper panel in Fig.5 shows the relative force error versus interparticle separation, given in the units of the base grid, for a pure PM calculation and for the second and fourth refinement levels. Note that despite the general similarity of the shape of FFT and relaxation forces, the scatter of the latter at small separations is larger. The relaxation force, however, is about twice "softer" (it reaches a $\approx 5\%$ error level only at separations ≈ 2 grid cells, the FFT force reaches this level at ≈ 1 cell). The scatter at small separations does not, however, mean that we have the same errors in particle orbits. In the case of a circular orbit with a radius of 3 cells, for example, the error in radius is less than 1% for at least a few orbital periods in both methods.

The lower panel in Fig.6 shows the relative error for ART force calculated on the fourth level versus distance in the units of the fourth level mesh cell together with the relative error corresponding to the Plummer softened force (solid line) with the softening parameter ϵ ($\phi \propto 1/\sqrt{r^2 + \epsilon^2}$) equal to the size of the fourth level cell. Comparison shows that while ART force fluctuates around zero for distances greater than two mesh cells, the Plummer softened force is considerably lower than $1/r^2$ law for up to six grid cells. The relation between resolution of the ART code, h_{ART} , and Plummer softening length is thus $\epsilon \approx 3h_{ART}$. Gelb (1992) studied the shape of the Plummer softened force in his P³M code. The result is consistent with ours (Fig. 2.4 in Gelb 1992) – the force starts to fall down at a distance about five times larger than the softening length.

⁸We should note that particles in the CIC scheme (see Section 2) have cubic rather than spherical shape so that the exact force at small separations is not an inverse square function of distance.

4.2. Zel'dovich' pancake collapse

The one-dimensional plane wave collapse in an expanding universe is one of the traditional tests of N-body codes (Klypin & Shandarin 1983; Efstathiou et al. 1985). In this test, the analytical solution (Zel'dovich 1970) is used to check how accurately the code integrates particle trajectories. If we know the initial conditions, the solution predicts particle positions for any other moment of time:

$$\mathbf{x}_i^Z = \mathbf{q}_i + \left(\frac{\mathbf{A}}{2\pi k}\right) \cos\left(2\pi \mathbf{k} \cdot \mathbf{q}\right),$$

here q_i are the initial (unperturbed) positions, k is the wavevector, and A(t) is the amplitude. In an $\Omega = 1$ universe, $A = a(t)/a_0$ where a_0 is scale factor at the crossing time. The corresponding velocities can be obtained by differentiating the above formula for positions.

We used a 32³ base grid with 64³ particles. The particle positions and velocities were initially perturbed using the Zel'dovich approximation. The particle trajectories were integrated by the ART code with three levels of refinement (the density threshold for opening the next level was twenty particles in a cell on the base grid and three particles in a cell for any refinement level). In Fig.7 we show one-dimensional phase diagrams at the crossing time where results of the ART code are compared with results of PM code (32³ grid). The figure shows that the ART code follows the analytical solution more accurately than the PM code. This is shown quantitatively in Fig.8, where we plot rms deviations of the particle positions and velocities from the exact solution as a function of time (Efstathiou et al. 1985): $\Delta x_{rms} = \left[\sum (x_i - x_i^Z)^2 / \sum (x_i^Z - q_i)^2\right]^{1/2}$, $\Delta v_{rms} = \left[\sum (v_i - v_i^Z)^2 / \sum (v_i^Z)^2\right]^{1/2}$. Starting from the moment when the first refinement level was created $(a \approx 0.29)$ the rms deviations were systematically lower in the ART code than in the PM code.

4.3. Spherical infall test

An analytical solution describing spherical infall of material onto an overdensity in an expanding cosmological framework was developed by Fillmore & Goldreich (1984) and Bertschinger (1985). As noted by Splinter (1996), the problem possesses a symmetry different from intrinsic planar symmetry of the mesh codes. This makes it a useful and strong test. The analytical solution describes the evolution of a spherical uniform overdensity $\delta \rho/\rho = \delta_i \ll 1$ in a region which has proper radius R_i at some initial time t_i in a flat Einstein-de Sitter universe. As the density contrast grows, the matter initially inside R_i is increasingly decelerated. Eventually it stops expanding and turns around to collapse. If the initial Hubble flow is unperturbed (all peculiar velocities are initially equal to zero), the initial turnaround occurs at the time t_{ita} :

$$t_{ita} = \frac{3\pi}{4} \delta_i^{-3/2} t_i.$$

At this moment the initial overdensity reaches its maximum radius:

$$r_{ita} = R_i \delta_i^{-1}.$$

Later on, shells of successively larger and larger radii turn around. At a given time $t \gg t_{ita}$, the shell of a radius

$$r_{ta}(t) = r_{ita} \left(\frac{t}{t_{ita}}\right)^{8/9}$$

starts to collapse (Bertschinger 1985).

The solution for the density profile of the overdensity is self-similar in terms of the dimensionless variable $\lambda \equiv r/r_{ta}(t)$ and for $\lambda \ll 1$ can be expressed as (Fillmore & Goldreich 1984; Bertschinger 1985):

$$D(\lambda) \approx 2.79 \lambda^{-9/4}$$

while at larger λ the main feature of the solution is the presence of sharp caustics.

We modelled the spherical infall problem described above by distributing 32^3 particles uniformly on the 32^3 grid (in the centers of the grid cells) and placing additional particles in a sphere of 2 grid cell radius in the center of the computational volume. The number of additional particles determines the initial overdensity that we have chosen to be $\delta_i = 0.2$. We integrated particle trajectories from $a_i = t_i^{2/3} = 0.1$ up to a = 10.1 making 10000 steps to insure that the Courant condition (i.e., particle moves only a fraction of a mesh cell in a single time step) is not violated on any of the five refinement levels – the condition required for the integration to be stable. The refinement levels were introduced in the regions where density was equivalent to more than six particles in a cell and the number of levels was limited to five making thus the effective resolution in the highest density regions equivalent to 1024. In Fig.9 the calculated density profile is compared with the analytical solution (from Tables 4 and 5 in Bertschinger 1985). We see a good agreement between the calculated density profile and the analytical solution at all radii down to the resolution limit.

4.4. Realistic cosmological runs: comparison with PM code

To test the performance of the code in realistic cosmological simulations we made a set of runs using ART and PM codes with the same initial conditions and different spatial resolutions and compared the resulting particle distributions. In the first four of runs we simulated an $L=20h^{-1}$ Mpc box with $N=32^3$ particles assuming a flat Λ CDM cosmological model ($\Omega_{\Lambda} = 0.7$, h = 0.7, $\sigma_8 = 1.0$). In ART runs we allowed for two levels of refinement starting from 643 and 1283 grids - we will call these runs ART 643+2L and ART $128^3 + 2L$. The number of time steps was ~ 1000 in the ART $64^3 + 2L$ and ~ 2000 in the ART $128^3 + 2L$ run. The refinement levels were introduced wherever the density exceeded a threshold value equivalent to more than 5 particles per cell. The PM code was run with 643 (PM 643) and 2563 (PM 2563) grids. In Fig. 10 we show the projected particle distribution at z = 0 from these four runs. The global distribution of particles and halos is well reproduced by the ART code. Also, halos in the ART 643 + 2L simulation are much more compact than in the PM 64³ simulation. This is shown quantitatively in Fig.11, where we compare density distribution functions (the fraction of the total mass in the regions of a given overdensity) in these simulations. The density distributions for all runs were computed after rebinning the density field to the 2563 grid. The resolution of a simulation puts limits on the maximum density in the halo cores because gravitational collapse virtually stops at scales of ~ 1 grid cell (e.g., Klypin 1996). Therefore, the density in the halo cores (the high-density tail of the distribution) is a good indicator of the spatial resolution. We note that the density distribution functions for both ART $64^3 + 2L$ and PM 256^3 runs show approximately the same behavior reaching overdensities of $\approx 2 \times 10^4$, while the PM 64³ run fails to produce halos with overdensities greater than $\approx 5 \times 10^3$. We, therefore, conclude that the ART code produces density fields similar to those of the PM code of comparable resolution.

The first application of the code was study of the structure of dark matter halos. Therefore, as a final test we compared the halo density profiles in the ART and PM simulations. The size of the simulation box, $L = 15h^{-1}$ Mpc, was chosen to be the same as in the larger simulations described in the next section.

The rest of the parameters were the same as in the above simulations. We simulated the evolution of the 32^3 particles using the PM code with 256^3 mesh and the ART code with a 64^3 base grid and three levels of refinement. As before, we refined regions where the local density exceeded a threshold value of about 5 particles per cell. A halo finding algorithm (described in the next section) was applied to the resulting particle distribution. In Fig.12 we present the density profiles for six halos of different masses. The mass resolution in these simulations $(1.2 \times 10^{10} M_{\odot})$ determined the mass range of halos. The most massive halo in Fig.11 consists of about 5000 particles while the least massive contains only about 100 particles. The density profiles of PM and ART halos agree reasonably well down to the resolution limit ($\sim 60h^{-1}$ kpc).

5. An application: structure of dark matter halos in CDM and ΛCDM models

5.1. Motivation

We used the code to study the structure of dark matter halos in two of the currently popular cosmological models – Standard Cold Dark Matter (SCDM) and Cold Dark Matter with cosmological constant (Λ CDM). The dark matter halos play a crucial role in the formation and dynamics of galaxies and galaxy clusters. Therefore, theoretical predictions about the structural and dynamic properties of the halos can be compared with observations and used as a powerful test of a given theoretical model. The numerical study of the halo structure requires very high spatial dynamic range (at least $\sim 10^4$) because the simulation box has to be large enough to account correctly for large perturbation waves and the force resolution has to be high enough to make predictions in the observational range (≤ 5 kpc). The ART code was designed to handle such high dynamic ranges.

The properties of dark matter halos were intensively investigated recently for a variety of cosmological models. Early numerical studies (Frenk et al. 1985; Quinn, Salmon, & Zurek 1986; Efstathiou et al. 1988; Frenk et al. 1988) indicated that the density profiles of dark matter halos in hierarchical clustering models in a flat, $\Omega = 1$, universe were approximately isothermal $(\rho(r) \propto r^{-2})$ in agreement with analytical results (Fillmore & Goldreich 1984; Bertschinger 1985). The dependence of the halo density profiles on the initial perturbation spectrum and on specific parameters of the cosmological model were also studied both analytically (Hoffman & Shaham 1985; Hoffman 1988) and numerically (e.g., Crone, Evrard, & Richstone 1994). These early numerical studies, however, lacked the necessary mass and spatial resolution to make reliable predictions on the structure of the halo cores. To overcome the resolution limits, substantial efforts were made to simulate the formation of halos from isolated density perturbations (e.g. Dubinski & Carlberg 1991; Katz 1991) or to resimulate with a higher resolution halos identified in large low-resolution runs (Navarro, Frenk, & White 1996; Tormen, Bouchet, & White 1996). These simulations have the advantage of simulating halos in a wide mass range with homogeneous spatial and mass resolutions. However, the tidal effects from the neighboring galaxies and effects of halo mergers are simulated rather roughly. It is therefore important to check the results of such simulations with the results of direct simulation of halo formation in a representative box. Studies of the structure and dynamics of halos extracted from high-resolution direct simulations were done by Warren et al. (1992) and Cole & Lacey (1996). Warren et al. (1992) used TREE code to simulate the evolution of 128^3 particles in an $\Omega = 1$ universe with scale-free initial conditions. The force resolution was determined by imposing a Plummer softening of $\epsilon=5$ kpc. A special emphasis was made on the investigation of halo shapes. Similar initial conditions were used in the study by Cole & Lacey (1996), who used a P³M code to evolve 128³ particles. The resolution in the latter simulations was $L/\epsilon = 3840$, where L is the size of the computational volume and ϵ is the Plummer softening parameter. The results

indicated that the density profiles of all simulated halos are well fit by the analytical model of Navarro, Frenk, & White (1996) (hereafter NFW). This model has $\rho \propto r^{-1}$ at small radii and steepens smoothly to $\rho \propto r^{-3}$ at a scale radius r_s :

 $\rho(r) \propto \frac{1}{r(1+r/r_s)^2}. (20)$

The density profile described by this expression is singular, because density rises arbitrarily high when $r \to 0$ forming a cusp. The cuspy structure of the central parts of a halo represents thus a generic prediction of the model. Although the NFW profile is consistent with current X-ray and gravitational lensing observations of galaxy clusters (NFW), the $\rho \propto r^{-1}$ behavior is in contradiction with observations of dynamics of dwarf spiral galaxies that imply flat central density profiles (Flores & Primack 1994; Moore 1994; Burkert 1996). These observations can serve as one of the critical tests of any model that includes a dark matter component because it is generally believed that the dynamics of the dwarf spiral galaxies is dominated by dark matter on scales $r \geq 1$ kpc. The fact that the NFW profile holds for a variety of cosmological models (NFW; Cole & Lacey 1996) indicates its possible universality for CDM-like models. The goal of the present study was to investigate the structure of dark matter halos formed in a Λ CDM model. This model is currently one of the most successful scenarios of structure formation in the Universe. It is, therefore, important to check whether the central cusp is present in halos formed in this model.

5.2. Simulations

To study the structure of dark matter halos we simulated the evolution of 64^3 particles in standard CDM ($\Omega=1,\,h=0.5,\,\sigma_8=0.63$) and ΛCDM ($\Omega=0.3,\,\Omega_{\Lambda}=0.7,\,\sigma_8=1.0$) models. We made three runs – one high-resolution (resolution $\sim 2h^{-1}$ kpc) run for each models, and a lower resolution run (resolution $\sim 8h^{-1}$ kpc) for the ΛCDM model to study the effects of resolution. In terms of the Plummer softening length (see Section 4.1), our resolution corresponds to $L/\epsilon\approx 12000$ for the high resolution runs, and $L/\epsilon\approx 3000$ for the low resolution run. The simulations were started at z=30 and particles trajectories were integrated by making 3872 time steps in the low resolution run, and 7743 time steps in high-resolution runs. The size of the simulation box, $L=15h^{-1}$ Mpc, determines the mass resolution (particle mass) – 1.523 × $10^9h^{-1}M_{\odot}$ for SCDM and $5.077 \times 10^9h^{-1}M_{\odot}$ for ΛCDM .

5.3. Halo finding algorithm

To identify halos in our simulations we use an algorithm similar to that described in Klypin, Primack, & Holtzman (1996). The algorithm identifies halos as local maxima of mass inside a given radius. The efficiency of the algorithm was improved by incorporating the idea of Warren et al. (1992) of finding approximate locations of density peaks using particle accelerations. This idea is based on the principle that particles with the largest accelerations should reside near the halo centers which is true for halos with roughly isothermal density profiles. In practice, this way of finding density maxima has proved to be quite efficient. The halo identification algorithm can be described as follows.

- 1. The particles are sorted according to the magnitude of their scalar accelerations.
- 2. The particle with the largest acceleration determines the approximate location of the first halo center. Particles located inside a sphere of radius r_{init} centered at the halo center are assigned to the same halo and are excluded from the list of particles used to identify halos. The radius r_{init} is an adjustable parameter;

we use a radius approximately twice larger than the force resolution of a simulation. The procedure repeats for the particle with the largest acceleration in the list of remaining particles. The peaks are identified until there are no particles in the list.

- 3. When all the density peaks are identified, we proceed to find more accurate positions of the halo centers. This is done iteratively by finding the center of mass of all particles inside r_{init} and displacing the center of the sphere to the center of mass. The procedure is iterated until convergence.
- 4. When the halo centers are found, we increase r_{init} until the overdensity inside the corresponding sphere reaches a certain limit. The limit is based on the top-hat model of gravitational collapse that predicts the typical overdensity for virialized objects ~ 200 in CDM and ~ 334 for our Λ CDM model (e.g. Lahav et al. 1991; Kitayama & Suto 1996). However, we denote halo radius and mass inside this radius defined as M_{200} and r_{200} regardless of the actual value of the limit. Smaller halos located within a radius r_{200} of a bigger halo are deleted from the list.

As an output we get a list of halo positions, velocities, and parameters (such as r_{200} and M_{200}).

5.4. Results: halo density profiles

We applied the halo finding algorithm described above to identify halos in the simulations at zero redshift. Only halos with more than 100 particles within r_{200} were taken from the full list. We also present results for relatively isolated halos, excluding all halos which have close $(r < 2r_{200})$ neighbors of mass more than half of the halo mass. The density profiles were constructed by estimating the density in concentric spherical shells of logarithmically increasing thickness with the smallest radius corresponding to the maximum resolution. The resulting profiles were fit (the fit parameter was the scale radius r_s) with the analytical formula of NFW (eq. 20). In Fig.13 and 14 we show density profiles of 9 halos of different mass identified in the high-resolution CDM and Λ CDM simulations along with the analytical fits. The NFW profile appears to be a good approximation for halos of all masses (within the mass range of our simulations) in both CDM and Λ CDM models.

NFW argued that the concentration parameter, $c = r_{200}/r_s$ (see eq.20), of a dark matter halo depends on the halo mass. They have found that low mass halos are more centrally concentrated than high mass ones which possibly reflects different formation redshifts of halos. Fig.15 shows the concentration c as a function of halo mass (M_{200}) for halos identified in our simulations. The solid curve represents a theoretical prediction (see NFW for discussion) assuming a definition for the formation time of a halo as the first time when half of its final mass M_{200} was in progenitors with individual masses exceeding fraction f = 0.01 of M_{200} . This particular value of f seemed to provide the best approximation to the numerical results of NFW for the CDM model. The results of both the CDM and the Λ CDM simulations agree reasonably well with this curve. The larger spread of parameter c for low mass halos is due largely to the statistical noise. The lowest mass halos $(M_{200} \sim 10^{11.5} \, \mathrm{M}_{\odot})$ contain a few hundred particles within their r_{200} and thus have more noisy density profiles (typical 2σ error in $\log c \sim 0.2 - 0.3$) compared to more massive halos $(M_{200} > 10^{13} \, \mathrm{M}_{\odot})$ which have tens of thousands of particles (error in $\log c \sim 0.05$).

5.5. Effects of resolution

It is important to model reliably the structure of the very central parts $(r < 10h^{-1} \text{ kpc})$ of a halo because that is where we can compare model predictions with observational results. Unfortunately, that is also where force resolution may strongly affect the shape of the density profiles. To study possible effects of resolution, we have compared density profiles of the same halos taken from Λ CDM simulations of different resolution described in Section 5.2. In Fig. 16 we compare density profiles of 4 halos from these simulations. As before, the density profile is drawn only to the resolution limit of simulation. We conclude that, up to the resolution limit, the lower resolution density profile follows that of the higher resolution simulation.

5.6. Conclusions

We studied the structure of dark matter halos in CDM and Λ CDM models with a resolution of $\sim 2h^{-1}$ kpc in a box of $15h^{-1}$ Mpc.

- 1. We found that for $r < r_{200}$, the density profiles of all halos in both CDM and Λ CDM simulations are well fit by the analytical formula (eq. 20) of Navarro et al. (1996).
- 2. The mass dependence of the halo concentration parameter c in our simulations is consistent with the results of Navarro et al. (1996).
- 3. The fact that our results for the CDM model agree with the results of Navarro et al. (1996) serves both as a final test of the presented code and as an independent check of their method with results from direct cosmological simulations.

6. Discussion and conclusions

We present a new high-resolution N-body code which incorporates the idea of Adaptive Refinement Tree (Khokhlov 1997) to build a hierarchy of refinement meshes in regions where higher resolution is desired. Unlike other N-body codes that make use of refinement meshes, our code is able to construct meshes of arbitrary shape covering equally well both elongated structures (such as filaments and walls) and roughly spherical dark matter halos. The meshes are modified to adjust to the evolving particle distribution instead of being rebuilt at every time step. We use a cubic grid as the zeroth level of the mesh hierarchy. The size of this grid determines the minimum possible resolution of a simulation (i.e., resolution in regions where there are no refinements). The code blocks working on the zero level grid are similar to those of a PM code. To solve the Poisson equation on refinement meshes we have developed a new solver that uses a multilevel relaxation method with Successive Overrelaxation (Hockney & Eastwood 1981; Press et al. 1992). The solver is fully parallel and is only ~ 2 times slower than an FFT solver for the same number of mesh cells. In real simulations with the same resolution, the relaxation solver outperforms the FFT because the resolution is achieved with much smaller number of cells (see Section 3.7) The presented tests (Section 4) show that our code adequately computes gravitational forces down to scales of $\sim 1.5-2$ mesh cells. The memory overhead in the current version of the code is rather large compared to other high-resolution codes. The number of required mesh cells, however, changes very slowly with increasing resolution. At present, the code is capable of handling a dynamic range as high as ~ 10000. Also, tests of the code performance show that it is about three times faster than an AP3M code (and thus TREE code, see Couchman 1991) of comparable resolution. Still, the Courant condition requiring that particles move only a certain fraction of a mesh cell at every time

step makes the code CPU rather than memory limited.

The present version of the code is by no means optimal and we plan the following improvements.

- 1. The memory requirement of the code can be significantly reduced if pointers that are used to support the tree refinement structure are shared by siblings (descendants of the same parent cell). The memory overhead can be reduced even further by incorporating more elaborate algorithms of data storage (Khokhlov 1997).
- 2. The current version of the code (as well as any other high-resolution code) is constrained by the Courant condition. To insure that this condition is satisfied on the maximum refinement level requires small time steps redundant for particles moving on coarser meshes. We plan to incorporate an integration scheme with multiple time steps.
- 3. We plan to integrate the present N-body code with a high-resolution Eulerian hydrodynamics code (Khokhlov 1997) which works on similar refinement meshes.

We have used the ART code to study the structure of dark matter halos in two cosmological models—standard CDM ($\Omega=1,\,h=0.5,\,\sigma_8=0.63$) and a variant of Λ CDM ($\Omega=0.3,\,\Omega_{\Lambda}=0.7,\,\sigma_8=1.0$). We have found that halos formed in Λ CDM model have density profiles similar to halos formed in CDM model. The density profiles are well described by the analytical formula (eq. 20) presented by Navarro et al. (1996) and have cuspy ($\rho(r) \propto r^{-1}$) structure in the central ($r < 10h^{-1}$ kpc) parts of a halo with no indications of a core down to the resolution limit of our simulations. We therefore conclude that halos formed in the Λ CDM model have structure similar to the CDM halos, and thus cannot explain dynamics of the central parts of dwarf spiral galaxies inferred from their rotation curves.

We would like to thank Almadena Chtchelkanova (Berkeley Research Associates, Inc.) for useful advices on various data structures and algorithms. We would like also to thank Gustavo Yepes, Michael Norman, and Michael Gross for fruitful discussions on various aspects of numerical simulations. We are grateful to Chris Loken for the help in improving the presentation of the paper. This project was supported in part by the grant AST9319970 from the National Science Foundation and by the Office of Naval Research. The simulations were done at the National Center for Supercomputing Applications (NCSA).

REFERENCES

Aho, A.V., Hopcroft, J.E., and Ullman, J.D. 1983, Data Structures and Algorithms (Reading: Addison-Wesley)

Anninos, P., Norman, M.L., and Clarke, D.A. 1994, ApJ 436, 11

Berger, M.J. 1986, SIAM J.Sci.Stat.Comput. 7, 904

Berger, M.J., and Colella, P. 1989, J.Comp.Phys. 82, 64

Berger, M.J., and Oliger, J. 1984, J.Comp. Phys. 53, 484

Bertschinger, E. 1985, ApJS 58, 39

Bouchet, F.R., and Hernquist, L. 1988, ApJS 68, 521

Brandt, A. 1977, Mathematics of Computation 31, 333

Burkert, A., 1996, ApJ 447, L25

Carrol, S.M., Press, W.H., and Turner, E.L. 1992, ARA&A 30, 499

Cole, S., and Lacey, C. 1996, MNRAS 281, 716

Corner, T.H., Leiserson, C.E., and Rivest, R.L. 1994, Introduction to Algorithms (New York: McGraw-Hill)

Couchman, H.M.P. 1991, ApJ 368, L23

Crone, M.M., Evrard, A.E., Richstone, D.O., 1994, ApJ 434, 402

Dubinski, J., and Carlberg, R.G. 1991, ApJ 378, 496

Efstathiou, G., Davis, M., Frenk, C.S., and White, S.D.M. 1985 ApJS 57, 241

Efstathiou, G., Frenk, C.S., White, S.D.M., and Davis, M. 1988 MNRAS 235, 715

Ferrell, R., and Bertschinger, E. 1994, Int.J. of Mod. Phys. C 5, 933

Fillmore, J.A., and Goldreich, P. 1984, ApJ 281, 1

Flores, R.A., and Primack, J.R. 1994, ApJ 427, L1

Frenk, C.S., White, S.D.M., Efstathiou, G., and Davis, M., 1985, Nature 317, 595

Frenk, C.S., White, S.D.M., Davis, M., and Efstathiou, G., 1988, ApJ 327, 507

Gelato, S., Chernoff, D.F., and Wasserman, I. 1996, ApJ submitted, preprint astro-ph/9607156

elb, J.M., 1992, PhD Thesis, M.I.T.

Gnedin, N.Y. 1995, ApJS 97, 231

Gnedin, N.Y., and Bertschinger, E. 1996, ApJ 470, 115

Gross, M. 1997, PhD Thesis (UCSC), in preparation

Hockney, R.W., and Eastwood, J.W. 1981, Computer simulations using particles (New York: McGraw-Hill)

Hoffman, Y. 1988, ApJ 328, 489

Hoffman, Y., and Shaham, J. 1985, ApJ 297, 16

Jessop, C., Duncan, M., and Chau, W.Y. 1994, J.Comp. Phys. 115, 339

Kates, R.E., Kotok, E.V., and Klypin, A.A. 1991, A&A 243, 295

Katz, N., 1991, ApJ 368, 325

Kitayama, T., and Suto, Y. 1996, ApJ 469, 480

Khokhlov, A.M., 1997, J.Comp.Phys., in preparation

Klypin, A.A., and Shandarin, S.F. 1983, MNRAS 204, 891

Klypin, A.A. 1996, Lecture notes at the International School of Physics "Enrico Fermi", S.Bonometto, J.R.Primack, and A.Provenzale (eds.), preprint astro-ph/9605183

Klypin, A., Primack, J., and Holtzman, J. 1996, ApJ 466, 13

Knuth, D. 1968, The Art of Computer Programming, Vol.1 (Reading: Addison-Wesley)

Lahav, O., Lilje, P.B., Primack, J.R., and Rees, M.J. 1991 MNRAS 251, 128L

Löhner, R., and Baum, J.D. 1991, AIAA paper 91-0620

Moore, B. 1994, Nature 370, 629

Navarro, J.F., Frenk, C.S., and White, S.D.M., 1996, ApJ 462, 563 (NFW)

Peebles, P.J.E. 1980, The Large Scale Structure of the Universe (Princeton: Princeton University Press)

Pen, U.-L. 1995, ApJS 100, 269

Press, W.H., Teukolsky, S.A., Vetterling, W.T., and Flannery, B.P. 1992, Numerical Recipes in FORTRAN, 2nd ed.

Quinn, P.J., Salmon, J.K., and Zurek, W.H., 1986, Nature 322, 329

Smith, C. 1995, Masters Thesis, NMT, Socorro

Splinter, R.J. 1996, MNRAS 281, 281

Suisalu, I., and Saar, E. 1995, MNRAS 274, 287

Suisalu, I., and Saar, E. 1996, MNRAS, submitted, preprint astro-ph/9511120

Tormen, G., Bouchet, F.R., White, S.D.M. 1996, MNRAS submitted, preprint astro-ph/9603132

Villumsen, J.V. 1989 ApJS 71, 407

Warren, M.S., Quinn, P.J., Salmon, J.K., and Zurek, W.H. 1992, ApJ 399, 405

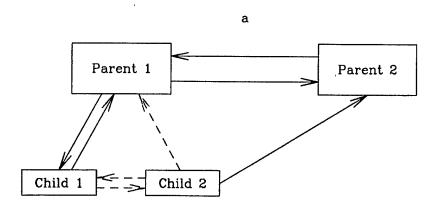
Wesseling, P. 1992, An Introduction to Multigrid Methods (New York: Wiley)

Xu, G. 1995, ApJS 98, 355

Yepes, G., Kates, R., Khokhlov, A., Klypin, A., 1996, MNRAS, in press

Zel'dovich, Ya.B., 1970, A&A 5, 84

This preprint was prepared with the AAS IATEX macros v4.0.



b

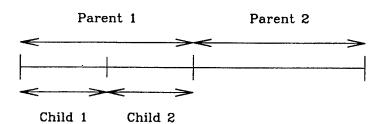


fig. 1

Fig. 1.— Schematic illustration of the tree structure and pointers used to support it in one dimension. Scheme (a) shows two neighbor cells (Parent and Neighbor) one of which (Parent) is split (it has two children denoted as Child1 and Child 2) and the other (Neighbor) is a leaf. The arrows denote pointers used to support the structure (see text for details). Arrows drawn with broken lines denote pointers which can be shared by all children. Below (b) we show the actual locations of the mesh cells in space.

fig. 2

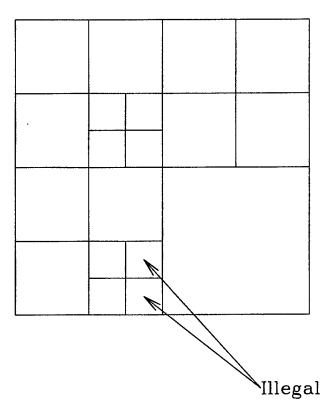


Fig. 2.— Examples of permitted and prohibited neighbor configurations. The prohibited configurations (the cells which violate the neighbor rule) are indicated with arrows. Note that it is not allowed to have neighbors with level difference greater than 1 but it is allowed to have a "corner neighbor" with level difference 2.

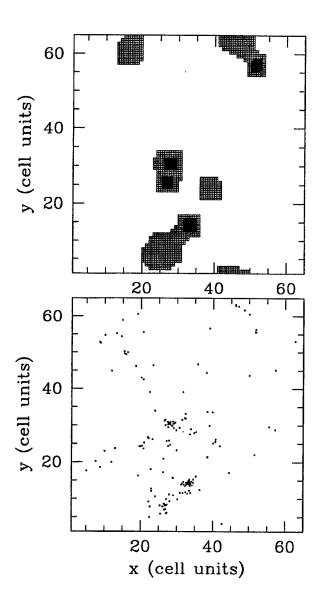


Fig. 3.— (a) A slice through the refinement structure (base grid is not shown) in one of the ΛCDM simulations with 32³ particles (see section 4.4) and (b) corresponding slice through the particle distribution. The square in (a) shows the area which is enlarged in Fig.4

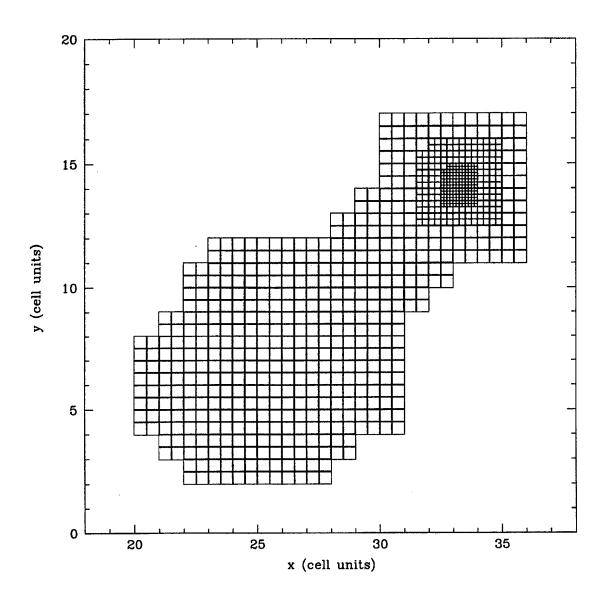


Fig. 4.— Fragment of the slice from Fig. 3a denoted by the square. Note that the mesh generator tends to build almost rectangular meshes around dense isolated clumps of particles while to trace a filament the generator creates meshes of arbitrary shape that effectively cover the elongated structures in particle distribution.

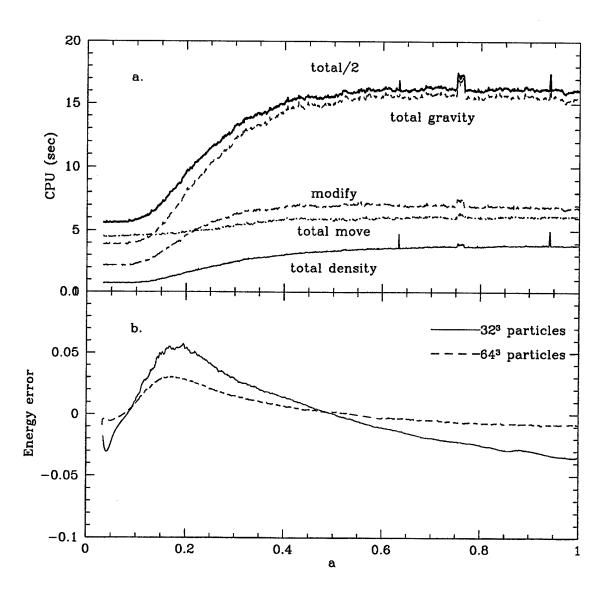


Fig. 5.— a) Timing for Λ CDM run with 32³ particles on 8 processors of SPP-1200 Exemplar (see section 3.8 for discussion). The total CPU time per step was scaled down by a factor of 2 for convenience. b) Energy conservation error versus expansion factor a in Λ CDM runs with 32³ (solid line) and 64³ (broken line) particles.

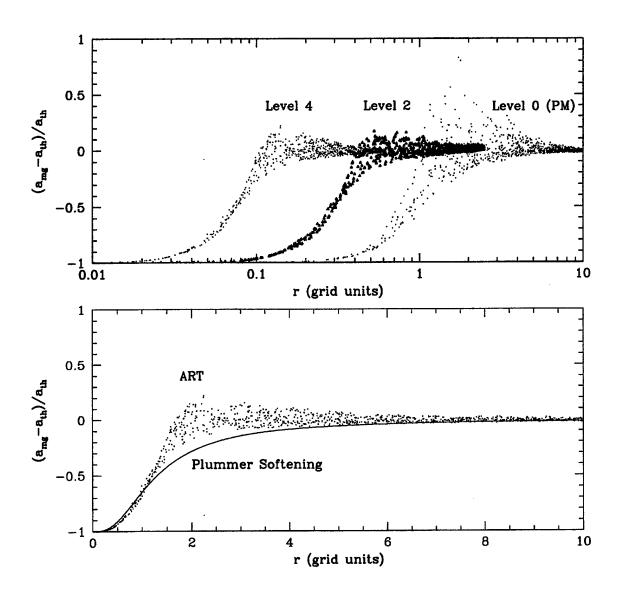


Fig. 6.— a) Pairwise force accuracy of the ART code on the base regular grid (FFT solver) and on the second and fourth refinement levels (relaxation solver) versus interparticle separation. b) Comparison of the force accuracy on the fourth refinement level with the theoretical accuracy of a Plummer softened force versus interparticle separation in units of the fourth level cells.

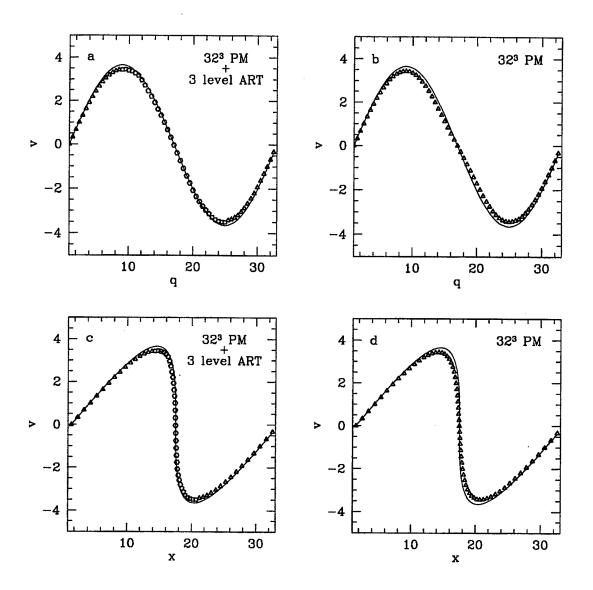


Fig. 7.— Plane wave collapse test: phase diagram in Lagrangian coordinates q with 3 refinement levels (a) and in PM simulation with 32^3 grid (b) at the crossing time. Solid line represents the analytical solution while polygons show numerical results. Number of polygon vertices is equal to the level plus three so that triangles show particles located on the base grid, squares show particles located on the first refinement level, and so on. The corresponding phase diagram for physical coordinates x are shown in panels x and x

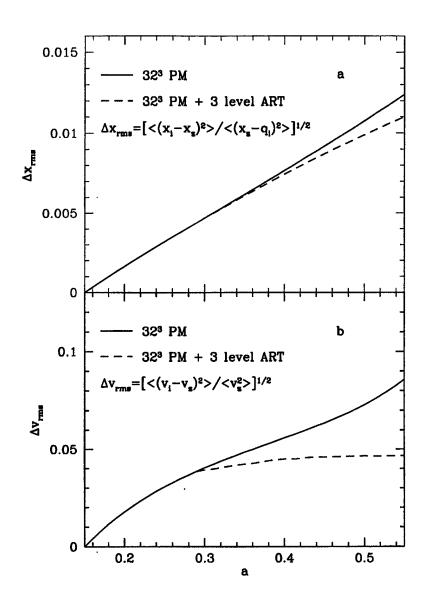


Fig. 8.— Plane wave collapse test: rms deviations of coordinates (a) and velocities (b) from analytical solution versus expansion parameter for PM code (solid line) and for ART code with three levels of refinement (broken line). Starting from the moment when the first refinement level was introduced ($a \sim 0.29$) the rms deviations in ART code are lower than in PM code

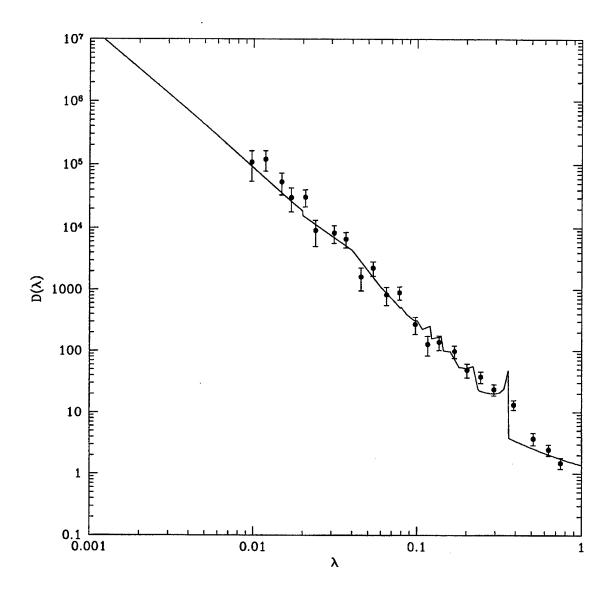


Fig. 9.— Spherical infall test: simulated density profile (filled circles) is compared with the analytical solution (solid line). The points for the analytical solution are taken from Tables 4 and 5 in Bertschinger (1985). The simulated density profile was constructed by estimating the density in concentric spherical shells of logarithmically increasing thickness with the smallest radius corresponding to the maximum resolution. The error bars correspond to the poisson noise.

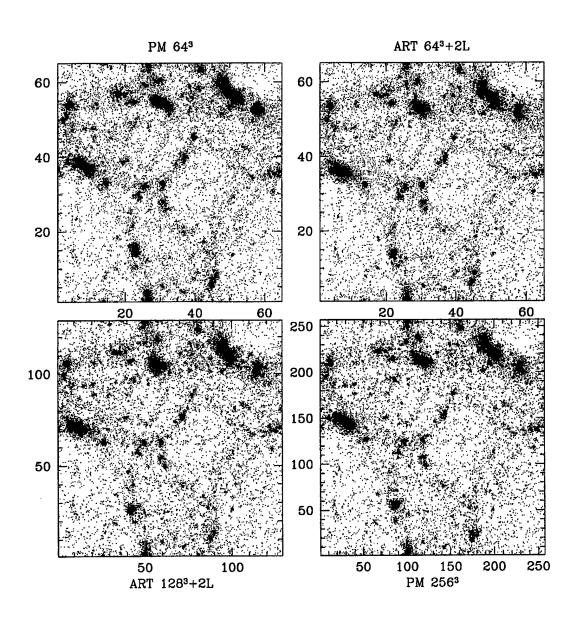


Fig. 10.— Comparison of projected final distributions of 32³ particles in pure PM runs with 64³ (a) and 256³ (d) grids and in ART runs with two levels of refinement and base grid of 64³ (b) and 128³ (c).

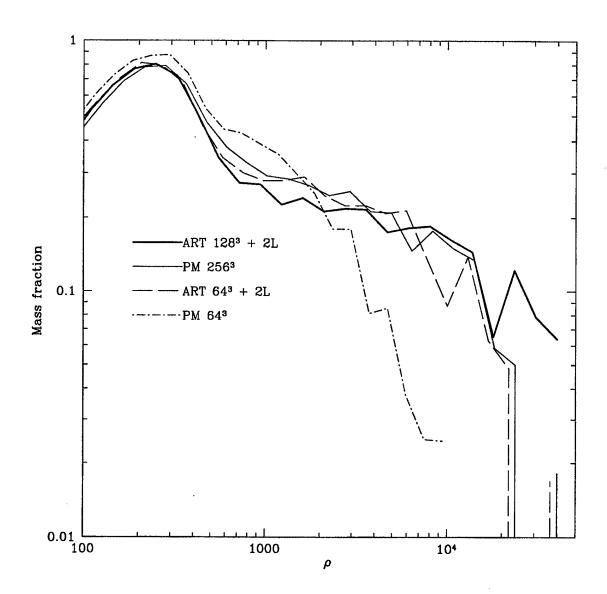


Fig. 11.— Comparison of density distribution functions (the fraction of the total mass in the regions of a given overdensity) for PM and ART (two refinement levels) runs. The density distributions for all runs were computed after rebinning the density field to the 256^3 grid. Note that the density distribution functions for both ART $64^3 + 2L$ and PM 256^3 runs show approximately the same behavior reaching overdensities of $\approx 2 \times 10^4$, whereas the PM 64^3 run fails to produce halos with overdensities greater than $\approx 5 \times 10^3$.

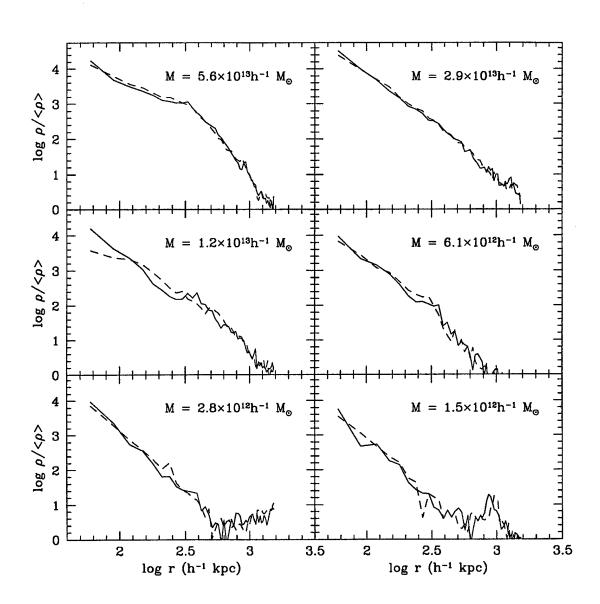


Fig. 12.— Comparison of density profiles for halos identified in PM (dashed lines) and ART (solid lines) simulations (32^3 particles) of comparable resolution ($\sim 60h^{-1}$ kpc) started from the same initial conditions.

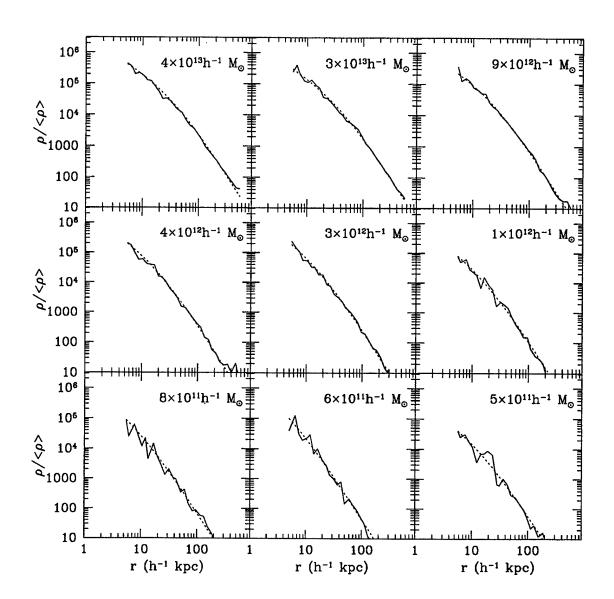


Fig. 13.— Density profiles (solid lines) for 9 halos of different masses taken from CDM simulation with 64^3 particles (resolution $\sim 2h^{-1}$ kpc) and the best fit of the analytical profile (dotted lines) of Navarro et al. (1996). The numbers indicate mass of a halo inside a radius corresponding to overdensity 200.

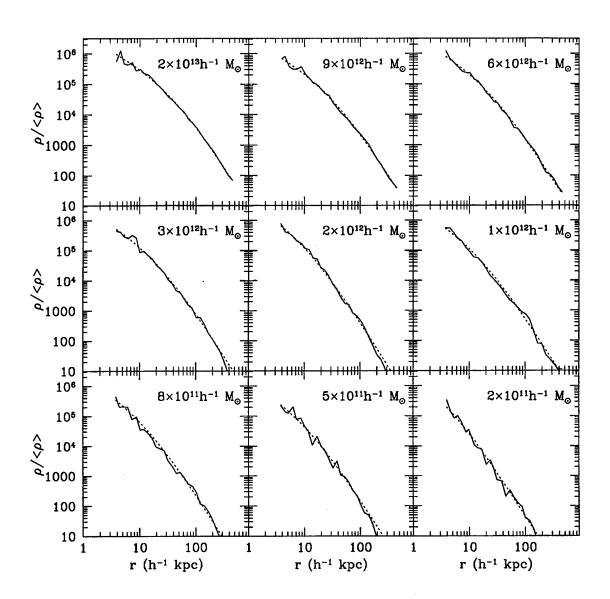


Fig. 14.— The same as Fig.13 for 9 halos of extracted from Λ CDM simulation (64³ particles, resolution $\sim 2h^{-1}$ kpc). The numbers correspond to a halo mass inside a radius of overdensity 334 (see Section 5.4).

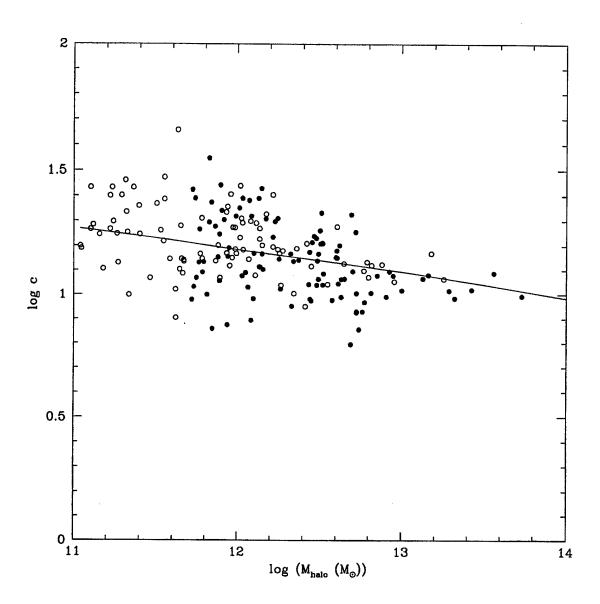


Fig. 15.— Logarithm of the concentration parameter, $c = r_{200}/r_s$, versus logarithm of halo mass M_{200} for high-resolution ($\sim 2h^{-1}$ kpc) CDM (filled circles) and Λ CDM simulations (empty circles). The solid curve shows the mass-concentration relation predicted from the formation times of halos which best described the numerical results of Navarro et al. (1996).

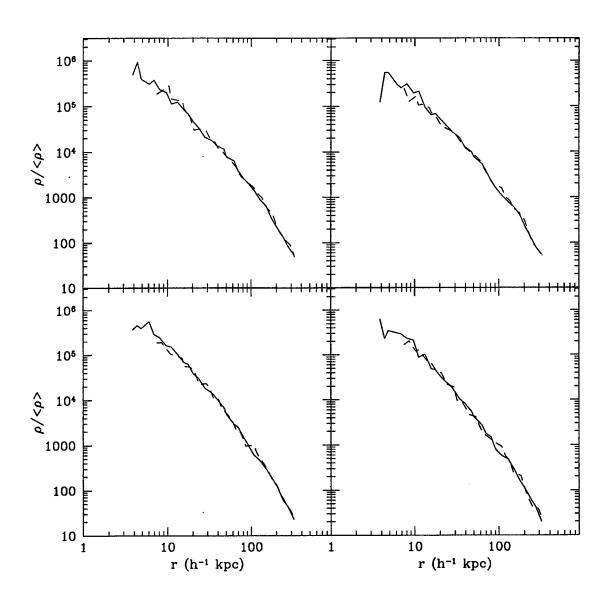


Fig. 16.— Effects of resolution on halo density profiles. The profiles of 4 halos taken from a Λ CDM run with $\sim 2h^{-1}$ kpc resolution (solid lines) and a run with $\sim 7h^{-1}$ kpc resolution (broken lines) are plotted down to the resolution limit.